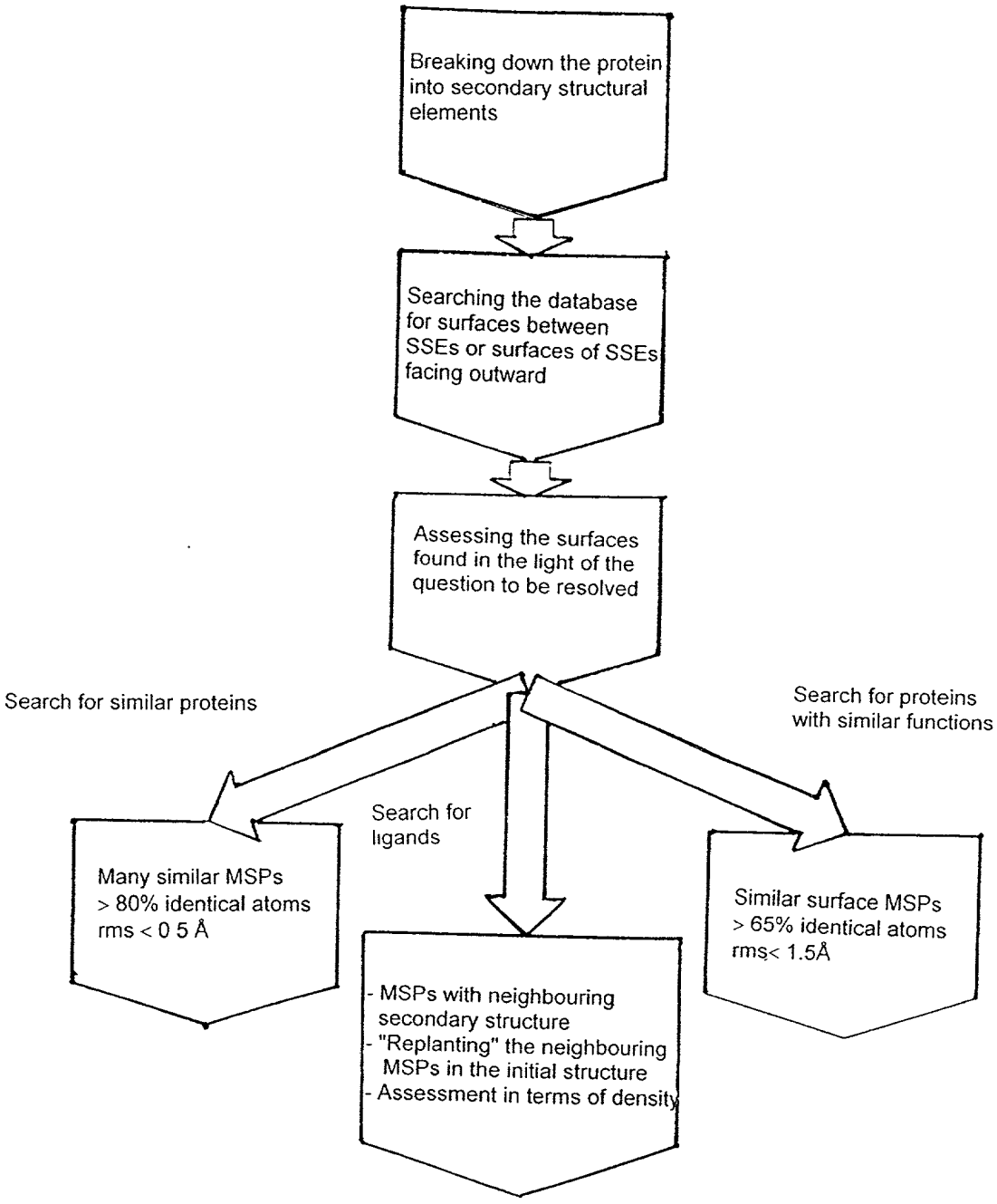

Breaking down the protein into secondary structural elements
Searching the database for surfaces between SSEs or surfaces of SSEs facing outward
Assessing the surfaces found in the light of the question to be resolved
Search for similar proteins
Search for ligands
Search for proteins with similar functions
Many similar MSPs
> 80% identical atoms
rms < 0 5 Å
- MSPs with neighbouring secondary structure
- "Replanting" the neighbouring MSPs in the initial structure
- Assessment in terms of density
Similar surface MSPs
> 65% identical atoms
rms< 1.5Å

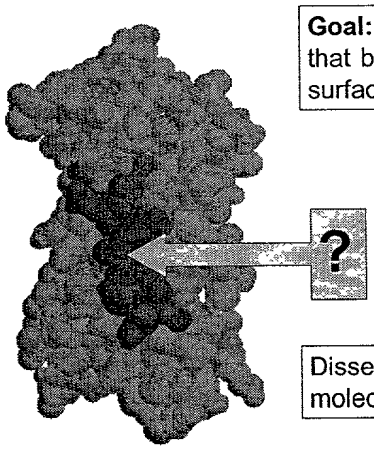
Fig. 1

The Principle of Ligand Identification

The Process

Dictionary of Interfaces in Proteins

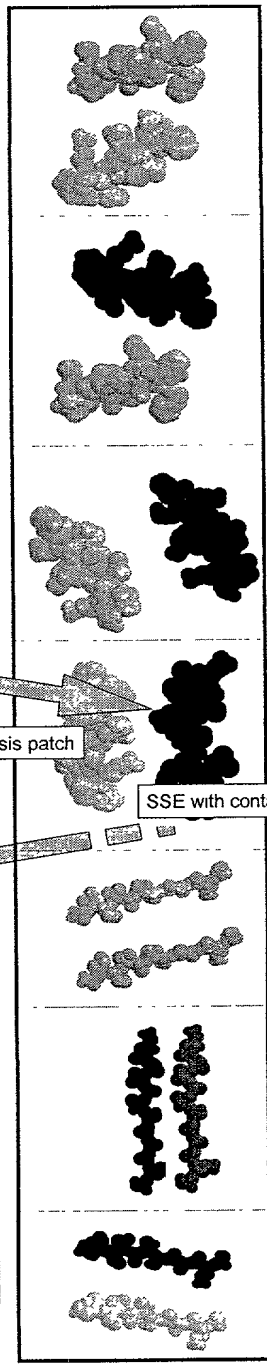
Goal: Identification of a ligand that binds to a predefined protein surface area (active site)



Dissection of the protein surface in molecular surface patches (MSPs)

Definition of MSP(s) forming the active site for which a ligand has to be identified

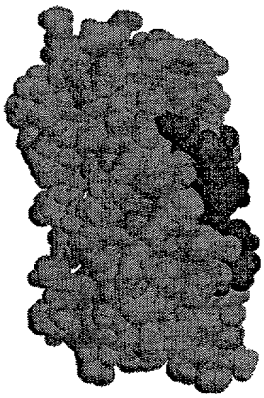
Search for MSPs (basis patches) in the databank that are similar to the active site MSP(s) with respect to geometric parameters and fitting atomic species



SSE with basis patch

SSE with contact patch

The contact patch is supposed to be complementary to the active site MSP.



Transformation of co-ordinates of the contact patch-SSEs on the active site MSP and evaluation of the fit by local atomic density [3].

Fig. 2

The „Dictionary of Interfaces in Proteins" (DIP) is a collection of interfaces that are defined as pairs of matching molecular surface patches between neighboring secondary structural elements. Each interface consists of two subsets of atoms from neighbouring secondary structure elements (pairs of complemetary MSPs). All such interfaces from known protein structures were collected in a comprehensive data bank (DIP).

Abbreviations:
SSE: secondary structual element
MSP: molecular surface patch